# ESRA Project Proposal Form

# Project title

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| Statistical Mechanics Project |

# Department(s)

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| --- |
| Physics |

# General information

*List the group members (starting with project leader, if you have one). Include year of study, email address and departmental affiliation:*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Name | Year of study | Student number | Email Address | Departmental Affiliation |
| Max Conneely | 3 | s2549354 | s2549354@ed.ac.uk | Physics |
| Edward Johnson |  | s2629954 | s2629954@ed.ac.uk | Physics |
| Nicolas Pisanello-Marshall |  | s2630700 | s2630700@ed.ac.uk | Physics |
| Griffin Spears |  | s2638547 | s2638547@ed.ac.uk | Physics |
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# Project Information

# *Description*

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| Many material properties of interest in Thermodynamics are bulk properties: emergent properties from the interactions of many particles. Mathematically, the bulk properties are defined as integrals over all the microstates of a statistical ensemble in equilibrium. Even in computer simulations with a few hundred particles, the Hamiltonian phase space of the system is quite high dimensional. To evaluate bulk properties, the Metropolis Monte Carlo method must be employed to integrate over the significant regions of the ensemble (importance sampling) instead of integrating over the entire system phase space. |

## 

## Aims

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| We aim to obtain an equation of state or a phase diagram for several different atomic or molecular interaction potentials. The two potentials of particular interest are the hard-sphere potential and the Lennard-Jones potential. We shall obtain the phase diagrams and equations of state using numerical methods. |

## Methodology

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| We shall be using the Metropolis Monte Carlo method for numerical integration over the system phase space due to its high dimensionality. We will likely use a discretised 3D grid where each particle has a Lennard-Jones potential and periodic boundary conditions are imposed to mimic bulk conditions. |

## Significance

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| None of this research is likely to produce novel results, however, it should familiarise people with numerical methods often used in high dimensional systems alongside some of the basic principles of statistical mechanics. |

## Lay summary

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| Unpredictability can arise in systems which are, at least in principle, predictable. The result of a die can in principle be predicted, however, the physics governing the die’s evolution in time results in the state of the die after some time to be highly sensitive to the die’s initial conditions leading to what is essentially a random outcome.  This phenomenon also appears in collisions of 3 or more snooker balls, and in the extreme case of many molecules interacting in a material, where what is in principle predictable appears to be governed by probability theory instead. Such large systems are better described using probability distributions, and the properties of the probability distributions define material properties such as temperature and pressure. These distributions can be produced in small computer simulations of a few hundred particles, and their properties investigated. |

# Practical details

## Budget breakdown

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| --- | --- |
| **Description** | **Cost (£)** |
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|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
| **Total**: |  |

## Proposed start date (DD/MM/YEAR):

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 1 | 5 | / | 0 | 1 | / | 2 | 0 | 2 | 6 |

## Estimated duration:

|  |
| --- |
| 1 Year |

## Safety and training required

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| N/A |

## Supervisors

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| N/A |

PLEASE SUBMIT THIS FORM IN PDF FORMAT AS SOON AS POSSIBLE. FINAL DEADLINE IS THE **15th OF January 2026**. SUBMIT TO DEPARTMENT HEAD.

Good luck!